

QUANTUM SPIN CHAINS WITH REGULARLY ALTERNATING BONDS AND FIELDS

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Abstract

We consider the spin- $\frac{1}{2}$ XY chain in a transverse field with regularly varying exchange interactions and on-site fields. In two limiting cases of the isotropic (XX) and extremely anisotropic (Ising) exchange interaction the thermodynamic quantities are calculated rigorously with the help of continued fractions. We discuss peculiarities of the low-temperature magnetic properties and a possibility of the spin-Peierls instability.

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It is generally known that there are a number of one-dimensional spin models for which in the translationally invariant (uniform) case an exact calculation of the thermodynamic quantities is possible. To this class belong the spin- $\frac{1}{2}$ XY models proposed by Lieb, Schultz and Mattis [1]. At present there are relatively large number of magnetic and ferroelectric compounds which may be described by these models. On the other hand, due to the progress in material sciences a study of the properties of quantum spin chains with regularly varying parameters (e.g., exchange interactions or on-site fields) attracts much interest during last years. As an example one may mention the layered materials with the well-pronounced one-dimensional character in their properties known as superlattices, which can be viewed as chains with regularly varying exchange interactions (see, e.g., [2]). In what follows we show how the thermodynamic properties of the regularly alternating one-dimensional spin- $\frac{1}{2}$ XY model in a transverse field can be examined rigorously in two limiting cases of the isotropic exchange interaction (transverse XX chain) and of the extremely anisotropic exchange interaction (transverse Ising chain). We discuss briefly the effects of regular alternation on the magnetic properties of the chains at zero temperature. We also comment on a possibility of the spin-Peierls instability in the considered chains.

We consider a ring of $N \rightarrow \infty$ spins $\frac{1}{2}$ described by the Hamiltonian

$$H = \sum_n \Omega_n s_n^z + 2 \sum_n (I_n^x s_n^x s_{n+1}^x + I_n^y s_n^y s_{n+1}^y) \quad (1)$$

concentrating on two limiting cases 1) of the isotropic exchange interaction $I_n^x = I_n^y = I_n$ (transverse XX chain) and 2) of the extremely anisotropic exchange interaction $I_n^x = I_n$, $I_n^y = 0$ (transverse Ising chain). We assume that the exchange interactions I_n and the on-site (transverse) fields Ω_n vary regularly along the chain with

period p (N is a multiple of p), i.e., $I_1\Omega_1 I_2\Omega_2 \dots I_p\Omega_p I_1\Omega_1 I_2\Omega_2 \dots I_p\Omega_p \dots$. To calculate the thermodynamic quantities of the spin model we map it onto a system of spinless (Jordan-Wigner) fermions with the Hamiltonian [1]

$$H = \sum_n \Omega_n \left(c_n^+ c_n - \frac{1}{2} \right) + \sum_n \left(\frac{I_n^x + I_n^y}{2} (c_n^+ c_{n+1} - c_n c_{n+1}^+) + \frac{I_n^x - I_n^y}{2} (c_n^+ c_{n+1}^+ - c_n c_{n+1}) \right). \quad (2)$$

The Hamiltonian (2) can be brought into the diagonal form $H = \sum_k \Lambda_k (\eta_k^+ \eta_k - \frac{1}{2})$ where Λ_k is the elementary excitation energy and η_k^+ , η_k are Fermi operators. Obviously, the diagonalization of the Hamiltonian for $p > 1$ becomes not trivial.

To find the thermodynamic quantities of the spin model it is sufficient to know either $\rho(E) = \frac{1}{N} \sum_k \delta(E - \Lambda_k)$ or $R(E^2) = \frac{1}{N} \sum_k \delta(E^2 - \Lambda_k^2)$ since the Helmholtz free energy per site can be written as follows

$$f = -\frac{1}{\beta} \int_{-\infty}^{\infty} dE \rho(E) \ln \left(2 \cosh \frac{\beta E}{2} \right) = -\frac{2}{\beta} \int_0^{\infty} dE E R(E^2) \ln \left(2 \cosh \frac{\beta E}{2} \right). \quad (3)$$

Consider first the transverse XX chain. We introduce the one-fermion Green functions $G_{nm} = G_{nm}(E)$ which satisfy the set of equations

$$(E - \Omega_n)G_{nm} - I_{n-1}G_{n-1,m} - I_n G_{n+1,m} = \delta_{nm} \quad (4)$$

and yield the required density of states $\rho(E) = \mp \frac{1}{\pi N} \sum_n \text{Im} G_{nn}^{\mp}$, $G_{nm}^{\mp} = G_{nm}(E \pm i\epsilon)$, $\epsilon \rightarrow +0$. One immediately notes that the continued fraction representation for the diagonal Green functions which follows from (4)

$$G_{nn} = \frac{1}{E - \Omega_n - \Delta_n^- - \Delta_n^+}, \quad (5)$$

$$\Delta_n^- = \frac{I_{n-1}^2}{E - \Omega_{n-1} - \frac{I_{n-2}^2}{E - \Omega_{n-2} - \dots}}, \quad \Delta_n^+ = \frac{I_n^2}{E - \Omega_{n+1} - \frac{I_{n+1}^2}{E - \Omega_{n+2} - \dots}}.$$

is extremely useful in the case of regularly varying parameters I_n , Ω_n since Δ_n^- , Δ_n^+ in (5) become periodic and can be evaluated exactly by solving quadratic equations.

We cannot proceed in the described manner for the transverse Ising chain because of terms $c_n^+ c_{n+1}^+$, $c_n c_{n+1}$ in (2). However, from [1] we know that to find the (real) coefficients $g_{kn} = \frac{1}{2} (\Phi_{kn} + \Psi_{kn})$, $h_{kn} = \frac{1}{2} (\Phi_{kn} - \Psi_{kn})$ of the canonical transformation $\eta_k = \sum_n (g_{kn} c_n + h_{kn} c_n^+)$ which diagonalizes the Hamiltonian (2) one should solve the set of equations

$$\Omega_{n-1} I_{n-1} \Phi_{k,n-1} + (\Omega_n^2 + I_{n-1}^2 - \Lambda_k^2) \Phi_{kn} + \Omega_n I_n \Phi_{k,n+1} = 0 \quad (6)$$

(and a similar set of equations for Ψ_{kn}). Eq. (6) coincides with a set of equations describing displacements of particles in a nonuniform harmonic chain with nearest neighbour interactions and Λ_k plays a role of oscillator frequency. We can find the distribution of oscillator frequencies squares $R(E^2)$ from the relation $R(E^2) =$

$\mp \frac{1}{\pi N} \sum_n \text{Im} \Gamma_{nn}^\mp$, $\Gamma_{nm}^\mp = \Gamma_{nm}(E^2 \pm i\epsilon)$, $\epsilon \rightarrow +0$ where the Green functions $\Gamma_{nm} = \Gamma_{nm}(E^2)$ satisfy the set of equations

$$(E^2 - \Omega_n^2 - I_{n-1}^2) \Gamma_{nm} - \Omega_{n-1} I_{n-1} \Gamma_{n-1,m} - \Omega_n I_n \Gamma_{n+1,m} = \delta_{nm}. \quad (7)$$

From (7) the following representation for Γ_{nn} may be derived

$$\begin{aligned} \Gamma_{nn} &= \frac{1}{E^2 - \Omega_n^2 - I_{n-1}^2 - \Delta_n^- - \Delta_n^+}, \\ \Delta_n^- &= \frac{\Omega_{n-1}^2 I_{n-1}^2}{E^2 - \Omega_{n-1}^2 - I_{n-2}^2 - \frac{\Omega_{n-2}^2 I_{n-2}^2}{E^2 - \Omega_{n-2}^2 - I_{n-3}^2} - \dots}, \\ \Delta_n^+ &= \frac{\Omega_n^2 I_n^2}{E^2 - \Omega_{n+1}^2 - I_n^2 - \frac{\Omega_{n+1}^2 I_{n+1}^2}{E^2 - \Omega_{n+2}^2 - I_{n+1}^2} - \dots}. \end{aligned} \quad (8)$$

Again for a periodic sequence of parameters I_n , Ω_n the continued fractions Δ_n^- , Δ_n^+ in (8) become periodic and can be evaluated exactly by solving quadratic equations.

To illustrate how the described approach works we consider the chains of period 1 (uniform chains). Then for the transverse XX chain one finds

$$\begin{aligned} \Delta_n^- &= \Delta_n^+ = \frac{1}{2} \left(E - \Omega \pm \sqrt{(E - \Omega)^2 - 4I^2} \right), \\ \rho(E) &= \begin{cases} \frac{1}{\pi} \frac{1}{\sqrt{-(E - \Omega - 2I)(E - \Omega + 2I)}}, & \text{if } (E - \Omega)^2 < 4I^2, \\ 0, & \text{otherwise.} \end{cases} \end{aligned} \quad (9)$$

For the transverse Ising chain the corresponding results read

$$\begin{aligned} \Delta_n^- &= \Delta_n^+ = \frac{1}{2} \left(E^2 - \Omega^2 - I^2 \pm \sqrt{(E^2 - \Omega^2 - I^2)^2 - 4\Omega^2 I^2} \right), \\ R(E^2) &= \begin{cases} \frac{1}{\pi} \frac{1}{\sqrt{-(E^2 - (\Omega - I)^2)(E^2 - (\Omega + I)^2)}}, & \text{if } (E^2 - \Omega^2 - I^2)^2 < 4\Omega^2 I^2, \\ 0, & \text{otherwise.} \end{cases} \end{aligned} \quad (10)$$

Formulas (3), (9), (10) reproduce the long known results, however, the described approach (formulas (3), (5), (8)) yields new results for the chains of longer periods. These calculations are more lengthy (although transparent) and therefore are omitted here (see [3, 4]).

Let us discuss the effects caused by regular nonuniformity which can be studied rigorously within the framework of the elaborated approach. We start from the transverse XX chain. Regular alternation of the Hamiltonian parameters leads to a splitting of the fermion band (see (2)) into several subbands. Since the (transverse) magnetization per site is $m = -\frac{1}{2} \int_{-\infty}^{\infty} dE \rho(E) \tanh \frac{\beta E}{2}$ one immediately observes the plateaus in the dependence m vs. Ω at zero temperature $\beta \rightarrow \infty$ (we assume $\Omega_n = \Omega + \Delta\Omega_n$) which are accompanied by the square-root singularities in the zero-temperature dependence (transverse) susceptibility χ vs. Ω . The number of plateaus does not exceed the period of alternation, the characteristic fields at which the plateaus

start and end up (and the singularities of χ occur) can be easily calculated from the density of states $\rho(E)$. Consider further the case of modulated exchange interactions $|I_{1,2}| = |I|(1 \pm \delta)$ ($0 \leq \delta \leq 1$ is the dimerization parameter) and constant field Ω . One may easily convince himself that the ground-state energy per site $e_0 = -\frac{1}{2} \int_{-\infty}^{\infty} dE \rho(E) |E|$ for $|\Omega| < 2|I|$ decreases sufficiently rapidly with increasing δ to provide a spin-Peierls dimerization. Moreover, the ground-state energy of the chains having longer periods of exchange interaction modulation obtained with the help of continued fractions allows one to examine the stability of the transverse XX chain with respect to more complicated lattice distortions.

Let us pass to the transverse Ising chain. Considering the case of modulated exchange interactions (e.g., of period 2) and constant field and using the strong-coupling approach arguments (i.e., assuming the smallest interaction to be equal to 0) [5] one immediately notes that no magnetization plateaus should be expected. However, using the continued fraction approach results one may show that a logarithmic singularity of χ may occur if $\Omega = \pm I$ ($p = 1$), $\Omega_1 \Omega_2 = \pm I_1 I_2$ ($p = 2$) etc. As a result the transverse Ising chain may exhibit ‘plateaus’ in the dependence m vs. Ω for sufficiently large deviations of fields $\Delta \Omega_n$. Moreover, in contrast to XX chain, the number of singularities of χ (and the number of ‘plateaus’) for given p depends on the values of Hamiltonian parameters. The direct calculation of the ground-state energy of the dimerized Ising chain in a constant transverse field shows that no spin-Peierls instability should be anticipated that is in agreement with general arguments about the Peierls mechanism. Note, however, that the transverse Ising chain is unitarily equivalent to the anisotropic XY chain without field [6]. The latter model for a special choice of parameters may become the isotropic XY model for which, as we know from the rigorous calculation, the spin-Peierls instability does occur.

To summarize, we have discussed an application of continued fractions for calculation of the thermodynamic quantities of the regularly alternating spin- $\frac{1}{2}$ transverse XX and Ising chains. We have briefly discussed the magnetic properties of such chains as well as their stability with respect to a lattice distortion due to the spin-Peierls mechanism.

References

- [1] E. Lieb, T. Schultz, and D. Mattis: *Ann. Phys.* **16** (1961) 407.
- [2] L. L. Gonçalves and J. P. de Lima: *J. Phys.: Condens. Matter* **9** (1997) 3447.
- [3] O. Derzhko, J. Richter, and O. Zaburanyi: *Physica A* **282** (2000) 495.
- [4] O. Derzhko: *J. Phys. A* **33** (2000) 8627.
- [5] O. Derzhko: *Ukrainian Journal of Physics* **46** (2001) 762.
- [6] H. Braeter and J. M. Kowalski: *Physica A* **87** (1977) 243.